Discovering Rare Behaviors of Stochastic Models using Decision Procedures

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Outline

• Introduction
• Problem definition
• State of the art
• Our solution
  • Basic idea
  • Algorithm
  • Results
• Conclusion and Future Work
Introduction

- Discovering rare behaviours of stochastic models is an unsolved challenge.

- Several Domains:
  - Biomedical Devices,
  - Intelligent Automobiles,
  - Autonomous Robots

Space Vehicle  Artificial Pancreas  Infectious Disease
Why Stochastic Models? - I

- Even when models are deterministic
- The environment is quite complex e.g. road conditions
  - Stochastic models capture the unpredictability of inputs to the embedded system.
Why Stochastic Models? - II

- Complex life-critical embedded systems
- Must be proved correct when interacting with fundamentally stochastic systems
  - Biochemical environment models are fundamentally stochastic
Why Stochastic Models? - III

Models of Complex “Intelligent” Software are inherently stochastic

- E.g. Computer Vision algorithms, Machine Learning, Voice Recognition, Feature Extraction
• 32,000 Americans diagnosed with Pancreatic Cancer yearly.
• Next generation vehicles (will) do lane tracking, etc.
• In 2007, Lehman made $4 billion in profits.

• Almost all of them will die!
• Modify user inputs “if necessary”?
• It lost $3 billion in the spring and then another $4 billion in the following summer.

• Bits and pieces of stochastic biochemical models available!
• Stochastic models of human behavior!
Why Study Rare Behaviors?

- Rare but interesting or important behaviors
  - formation of a tumor,
  - spreading of infectious diseases,
  - failure of cyber-physical system
Stochastic Model Simulation

**Stochastic Model:**

- Naturally equipped with a well defined probability space.
- Example: DTMCs, CTMCs, **SDEs**
  - Deterministic Simulink Models with probabilistic inputs
  - Probabilistic Simulink Models
- Not an example:
  - Markov Decision Processes
  - C Programs
  - Digital Circuits
The form of a typical SDE:
\[ dX = b(t, X) \, dt + v(t, X) \, dW \]
where
- \( X \) is a system variable
- \( b \) is Riemann integrable function
- \( v \) is Ito integrable
- \( W \) is Brownian Motion
Why SDE models?

- Model dynamics of complex “less understood” systems.

- Investigation of biological phenomena and cyber-physical systems
  - sensitive to stochastic effects.
Behavioral Specification $\phi$ should be decidable on a finite sample trace of the model $M$.

- **Example:**
  - Bounded Linear Temporal Logic
  - Finite State Machine Specifications
  - “Sun will rise in the east within 24 hours”

- **Not an example:**
  - “Eventually, the sun will rise in the west some day.”
Statistical Model Verification

- Samples $X_i$ should be independent and identically distributed (i.i.d.) according to the model $M$.
  - $X_i = 1$ if the sample satisfies specification $\varphi$; 0 otherwise.

- Example:
  - i.i.d. random sampling of Simulink models

- Not an example:
  - Rare event simulation.
  - Symbolic Testing Strategies
Statistical Model Verification

Model M → Sample Traces → Behavioral Spec. \( \phi \) → MC Algorithm

Probability Threshold \( \rho \)

True → False
State of the Art: Statistical

- **Statistical Estimation:**
  - Given samples from a stochastic system,
  - Compute the probability that a system satisfies a given property.

- **Statistical Hypothesis Testing:**
  - Given a required confidence in the answer and a threshold probability
  - Draw as many samples as needed to decide
    - whether a stochastic system satisfies a given property with at least a threshold probability?

- Both approaches are really useless for rare but interesting behaviors
State of the Art: Statistical

- Use Girsanov’s theorem to change probability measures and then use statistical sampling to explore rare behaviors

- Sumit K. Jha and Christopher Langmead
  Understanding rare behaviors in stochastic biological models
  Best Paper at IEEE International Conference on Computational Advances in Bio and Biomedical systems
  Journal Version: BMC Bioinformatics

- Tries to explore rare behaviors but not a given rare behavior
Our New Approach - I

SDE Model

Behavioral Specification

Behavior Exploration Algorithm

Theoretical Results

Rare Behavior

SMT
Our Approach – II (RESERCHÉ)

Behavioral Spec. $\varphi$

SDE Model

Bit-Vector SMT formula $\mathcal{B}(\varphi)$

Bit-Vector SMT formula $\mathcal{B}(\text{SDE})$
Our Approach – II (RESERCHER)

Behavioral Spec. $\varphi$

SDE Model

Bit-Vector SMT formula (SDE)

Behavioral Spec. formula ($\varphi$)

Bit-Vector SMT formula
Our Approach – II (RESERCHE)

Behavioral Spec. \( \varphi \) → Bit-Vector SMT formula (\( \varphi \)) → Bit-Vector SMT formula (SDE) → Bit-Vector SMT formula

- Initial Values of Variables
- Max. time of simulation
- No. of simulation steps
Our Approach – II (RESERCHER)

Behavioral Spec. $\phi$

SDE Model

Bit-Vector SMT formula ($\phi$)

Bit-Vector SMT formula (SDE)

$P_{min}$, Lowest Prob. Density Behavior acceptable as witness to $\phi$

Initial Values of Variables

Max. time of simulation

No. of simulation steps
Our Approach – II (RESERCHE)

Behavioral Spec. $\phi$

SDE Model

Bit-Vector SMT formula ($\phi$)

Bit-Vector SMT formula (SDE)

Initial Values of Variables

Max. time of simulation

No. of simulation steps

$P_{\text{min}}$, Lowest Prob. Density

Behavior acceptable as witness to $\phi$

No feasible behavior found with prob. density $P_{\text{min}}$ or more

SMT Solver
Our Approach – II (RESERCE)

Behavioral Spec. $\phi$

SDE Model

Bit-Vector SMT formula ($\phi$)

Bit-Vector SMT formula (SDE)

Initial Values of Variables
Max. time of simulation
No. of simulation steps

$P_{\text{min}}$, Lowest Prob. Density Behavior acceptable as witness to $\phi$

SMT Solver

No feasible behavior found with prob. density $P_{\text{min}}$ or more

Feasible behavior satisfying $\phi$ found and print model
Our Approach - III

• SDE to Bit-Vector SMT formula

• Discrete Difference Equation

\[
\bigwedge_{k=0}^{m-1} \left( X_{t_{k+1}} = X_{t_k} + b(t_k, X_{t_k})(t_{k+1} - t_k) + v(t_k, X_{t_k}) \Delta W_{t_{k+1} \leftrightarrow t_k} \right)
\]

• $\Delta W$ is increment in Brownian motion
  – Normally distributed
  – with mean 0
  – and variance 1

• $t_{k+1} - t_k$ is increment in time
Intuitive Argument

• Large values of Brownian motion increments
  ➔ smaller probability densities
• Small values of Brownian motion increments
  ➔ large probability densities

A behavior has high probability density if it corresponds to small values of Brownian motion increments
Intuitive Argument

- Large values of Brownian motion increments
  ➔ smaller probability densities
- Small values of Brownian motion increments
  ➔ large probability densities

A behavior has high probability density if it corresponds to small values of Brownian motion increments.

Ask a decision procedure if there is a behavior satisfying the given specification with small values of Brownian motion increments.
Digging Deeper...

• The probability density of observing the value $X_{t_1}$ after $t_1$ time:

$$P(X_{t_1}|X_{t_0}) = P \left( W_{t_1} - W_{t_0} = \widetilde{W}_{t_1} - \widetilde{W}_{t_0}|X_{t_0} \right)$$

$$= P \left( W_{t_1} - W_{t_0} = \widetilde{W}_{t_1} - \widetilde{W}_{t_0}|W_{t_0} = \widetilde{W}_{t_0} \right)$$

$$= \frac{1}{\sqrt{2\pi(t_1 - t_0)}} e^{-\left(\frac{|W_{t_1} - W_{t_0}|^2}{2(t_1 - t_0)}\right)}$$

• Our results rely on
  • the independence of increments of Brownian Motions, and
  • their Gaussian distribution.
Digging Deeper… …

- We compute the probability density of observing the sequence of the observed discretized solution given the initial value:

\[
P(X_{t_0}, X_{t_1}, \ldots, X_{t_m} | X_{t_0}) \\
= P(X_{t_1}, \ldots, X_{t_m} | X_{t_0}) P(X_{t_0} | X_{t_0}) \\
= P(X_{t_2}, X_{t_3}, \ldots, X_{t_m} | X_{t_0}, X_{t_1}) \quad \text{Since, } P(X_{t_0} | X_{t_0}) = 1 \\
= P(X_{t_2}, \ldots, X_{t_m} | X_{t_0}, X_{t_1}) P(X_{t_1} | X_{t_0}) \\
= P(X_{t_2}, \ldots, X_{t_m} | X_{t_1}) P(X_{t_1} | X_{t_0}) \quad \text{Since, } P(X_{t_2} | X_{t_0}, X_{t_1}) = P(X_{t_2} | X_{t_1}) \\
= P(X_{t_3}, \ldots, X_{t_m} | X_{t_1}, X_{t_2}) P(X_{t_2} | X_{t_1}) P(X_{t_1} | X_{t_0}) \\
= \ldots \quad \ldots \quad \ldots \\
= P(X_{t_m} | X_{t_{m-1}}) \ldots P(X_{t_1} | X_{t_0}) \\
\quad - \frac{m}{2\Delta} \left( \sum_{i=1}^{m} (\overline{W}_t - \overline{W}_{t-1})^2 \right) \\
= (2\pi)^{-m/2} \Delta^{-m} e^{-\frac{1}{2}}
Digging Deeper… …

- We compute the probability density of observing the sequence of the observed discretized solution given the initial value:

\[ P(X_{t_0}, X_{t_1}, \ldots X_{t_m} | X_{t_0}) \]

\[ = P(X_{t_1}, \ldots X_{t_m} | X_{t_0}) P(X_{t_0} | X_{t_0}) \]

\[ = P(X_{t_1}, X_{t_2}, \ldots X_{t_m} | X_{t_0}, X_{t_1}) \quad \text{Since, } P(X_{t_0} | X_{t_0}) = 1 \]

\[ = P(X_{t_2}, \ldots X_{t_m} | X_{t_0}, X_{t_1}) P(X_{t_1} | X_{t_0}) \]

\[ = P(X_{t_2}, \ldots X_{t_m} | X_{t_1}) P(X_{t_1} | X_{t_0}) \quad \text{Since, } P(X_{t_2} | X_{t_0}, X_{t_1}) = P(X_{t_2} | X_{t_1}) \]

\[ = P(X_{t_3}, \ldots X_{t_m} | X_{t_1}, X_{t_2}) P(X_{t_2} | X_{t_1}) P(X_{t_1} | X_{t_0}) \]

\[ = \ldots \quad \ldots \quad \ldots \]

\[ = P(X_{t_m} | X_{t_{m-1}}) \quad \ldots \quad P(X_{t_1} | X_{t_0}) \]

\[ = (2\pi)^{-m/2} \Delta^m e^{-\frac{m}{2\Delta} \left( \sum_{i=1}^{m} \left( \tilde{W}_{t_i} - \tilde{W}_{t_{i-1}} \right)^2 \right)} \]

- We need to minimize the sum of squares of Brownian motion increments!
A key concern in discretizing SDE is the error introduced by sampling a continuous system and replacing a SDE with a discretized difference equation.

The existence and uniqueness of SDE ensures that the solution of an infinitely discretized SDE is the solution of the continuous SDE.

What is sufficiently discretized?
- 100, 1000, 10^4, ..., 10^100
- Stochastic mean value theorem and rate of convergence for various drift and diffusion.
Does a point lie on the trajectory of an ODE?
  - Not answerable in general
  - Works in practice; Lipschitz Continuity

Does a point lie on some path of a SDE?
  - Yes

Discretizing ODEs is fine with knowledge of Lipschitz constants
Discretizing SDEs is fine with knowledge of Lipschitz constants for drift and diffusion
Case Study – High Level View

Will 40% of the population be infected by malaria with 99% chance within 10 days?

Yes and here is the suggested control measures.

A high level view of our system: A person interacting with our system through web interface and our system is providing the instant results to the queries.
SARS: The number of infected people vs. Time plot.

Above prob. density is calculated when the number of infected people is more than 150 and less than 200 at the end of 40 time steps. Initially, no of infected people = 1

\[
\ln(\text{prob. density}) = -2.4 \times 10^8
\]
Experiments - II

SARS: The number of infected people vs. Time plot.

No. of time steps = 200
Case Study – High Level View

Will 40% of the population be infected by malaria with 99% chance within 10 days?

Yes and here is the suggested control measures..

A high level view of our system: A person interacting with our system through web interface and our system is providing the instant results to the queries.
Conclusion

- Algorithm for efficiently investigating rare behaviors in SDE models.
  - It avoids the computational costs associated with sampling
    - by searching for trajectories from the model that satisfy a given behavioral specification.
  - Only generates trajectories that exhibit the behavior.

- Our method takes advantage of the efficiency and power of the modern SMT-solvers.
Future Work

• Studying the use of decision procedures to analyze closed form solutions to SDEs.
  • Many practical applications require the study of the system where one component is SDE and the other component is a finite state controller.
    – Biologically important cyber-physical systems like artificial pancreas.
• Specialized decision procedures
  • Sum of Squares
  • Grobner Bases
  • Nonlinear SMT
• Extensive parallelization.
Future Work

- Integrated Circuit Performance
- Artificial Pancreata
- Computational Finance
- Autonomous Vehicles
Synthetic Biology

Genetic Similarity – Phenotypic Diversity
Synthetic Biology

FlavrSavr – Evolving away from synthetic target